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MODELING PBX 9501 OVERDRIVEN RELEASE EXPERIMENTS

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We show the failure of the standard Jones-Wilkins-Lee (JWL) equation of state (EOS) in modeling the overdriven release experiments of PBX 9501. The deficiency can be tracked back to inability of the same EOS in matching the shock pressure and the sound speed on the Hugoniot in the hydrodynamic regime above the Chapman-Jouguet pressure. After adding correction terms to the principal isentrope of the standard JWL EOS, we are able to remedy this shortcoming and the simulation was successful.

INTRODUCTION

High Explosives (HE) performs work by the expansion of its detonation products. Along with the propagation of the detonation wave, the equation of state (EOS) of the products determines the HE performance in an engineering system. The expansion typically begins at the Chapman-Jouguet (CJ) state and follows the principal isentrope to lower pressure. Since most theoretical EOS works cannot provide an accurate description of the principal isentrope as demanded in some applications, experiments are the only ways to extract the EOS information. The cylinder test approximates that condition and is perhaps the most commonly used method for the purpose. But it is doubtful that the EOS so obtained is still adequate in other conditions, particularly when pressure above CJ, known as the overdriven regime, is encountered. In an engineering device, the expansion cannot always be considered isentropic all the way and everywhere. The major factor is the system configuration. For example, the ideal process can be disturbed by wave reflection from various material boundaries causing the expansion to be interrupted by recompression. Also, the result of detonation waves interaction can lead to expansion beginning at pressure above CJ. In this paper, we will show how a standard JWL EOS fails to match the Hugoniot data and sound speed in that region and how we can improve the EOS with new correction. Finally, we show the success of the new EOS to simulate overdriven release experiments in which the detonation products pressure is maintained and then the expansion begins at pressure above the CJ.

JWL EQUATION OF STATE

The Jones-Wilkins-Lee (JWL) EOS[1] is perhaps the most popular form used in the HE community for a large class of problems but its nonuniquess is also well recognized. One of the problems is the variability of the CJ state, particularly the CJ pressure. We can attribute the variation to the reaction zone effect,[2] not the problem associated with the true products EOS. But even with the reaction zone taken care of, we have yet to claim the right JWL EOS is available for all problems.

The JWL form is essentially an emphirical-based EOS with the parameters determined mostly from the cylinder test, its validity is questionable in other hydrodynamic regime as mentioned. The overdriven Hugoniot pressure is such a quality useful for checking the EOS for the purpose. Experimental overdriven Hugoniot data have been available for sometime[3] and the JWL EOS has been shown to always underestimate the result .[4] The comparison of the recently available data for PBX 9501 (95%

HMX, 2.5% Estane, 2.5% BDNPA/BDNPF)[5] and the calculation based on a standard JWL EOS[6] in the overdriven regime shows similar trends. The difference is more pronounced further away from the CJ-state.

Another piece of important information is the sound speed, also recently made available experimentally.[5] Again, a substantial difference is observed and the calculated sound speed is much lower at higher pressure. To compensate for the deficiency of the conventional JWL EOS, more exponential terms can be added[7] but in doing so the original parameter set is perturbed. A new formulation is proposed in this work. It should be noted that no uniqueness can be proven in any of the empirical formulation however.

MODIFIED JWL EQUATION OF STATE

We add a correction to the conventional JWL expression to cover the high pressure region only while keeping the low pressure portion unchanged. The dividing line is the CJ state, more specifically, the CJ volume. In doing so we can preserve the utility of the original JWL parameters which are not upset by the new addition. Following the Grüneisen formulation,

$$p = p_i + \frac{\Gamma}{v}\left(\varepsilon - \varepsilon_i\right). \tag{1}$$

p is the pressure, ε the internal energy, and v the relative volume. Subscript i refers to the quantity on the principal isentrope. A different Grüneisen parameter representation Γ is used here for the reason given later. The new expressions for the pressure and the internal energy on the principal isentrope are:

$$p_i = \left[1 + F_p(v)\right] A\, e^{-R_2 v} + B\, e^{-R_2 v} + C\, v^{-(1+\omega)} \tag{2}$$

$$\varepsilon_i = \left[1 + F_\varepsilon(v)\right]\frac{A}{R_1} e^{-R_1 v} + \frac{B}{R_2} e^{-R_2 v} + \frac{C}{\omega} v^{-\omega} \tag{3}$$

A type of compressibility factor is applied to the high pressure exponential term. A polynomial form is chosen for simplicity with the reference point at the CJ volume v_{cj}. We intent to maintain a continuity in pressure as well as in sound speed and that is why the form is selected. The correction applies only when the volume is less than the CJ volume. The correction term for pressure is:

$$F_p(v) = A_0\left(v_{cj} - v\right)^2 + B_0\left(vcj - v\right)^3 \tag{4}$$

and for the internal energy,

$$F_\varepsilon(v) = \left(A_0 - \frac{3B_0}{R_1}\right)\left\{\frac{2}{R_1^2}\left[1 - e^{-R_1\left(v_{cj} - v\right)}\right] - \frac{2}{R_1}\left(v_{cj} - v\right) + \left(v_{cj} - v\right)^2\right\} + B_0\left(v_{cj} - v\right)^3 \tag{5}$$

There is no additional parameter introduced here since we have applied the isentropic relationship between the pressure and the internal energy and the new constants appearing in the pressure correction term also show up here. The continuity in the internal energy is thus maintained.

The calibration procedure is as follows. First we choose a Grüneisen parameter. For PBX 9501, we begin with Γ=0.38, the regular value of ω,[6] and fit the Hugoniot data above the CJ. The constants A_0 and B_0 are thus obtained. However, we notice that any reasonable choice of Γ is also acceptable to fit the Hugoniot data alone, the difference is in the values of A_0 and

B_0, and of course, the resulting isentrope which could be closer or farther from the Hugoniot, depending on the value of Γ. So the second stage is to check whether the selected constants A_0 and B_0 and the chosen Γ can fit the sound speed, a new feature in this work. Not a surprise to us, the standard value of 0.38 seems to be a reasonable one. A different approach based solely on the sound speed in the overdriven region leads to a slightly higher value, 0.45 and also a different value of CJ pressure, 355 kbar.[5] So it seems reasonable that Γ should vary from 0.38 to 0.45 as the volume decreases and that is the reason why we use a different symbol. We will include a volume dependence in Γ for the future work but for now, a constant of 0.38 is found adequate for PBX 9501. Figures 1 and 2 show both the original JWL EOS and the final modified JWL EOS results for the overdriven Hugoniot pressure and sound speed.

OVERDRIVEN RELEASE EXPERIMENT AND MODELING

A brief description of the overdriven release experiment is given here. A piece of sample HE is initiated by a high speed flyer. The HE is not only initiated but also maintained at pressure above the CJ value for a period of time at a given position until the rarefraction wave from the back of the flyer reaches the same location. The information is recorded by measuring the particle velocity between the HE and a transparent window. The velocity-time history shows the constant overdriven state. As the release waves moves in, the expansion begins at a pressure above the CJ state. The experiment we are to simulate uses an aluminum flyer of 4.711 mm thick impacting on the PBX 9501 at a velocity of 5.414 mm/μs. This provides an overdriven condition at pressure about 520 kbar. The HE thickness is 13.108 mm and at the end a transparent window of LiF is placed. The experimental result and the two different calculations, one with the standard JWL parameters alone and another with the modified

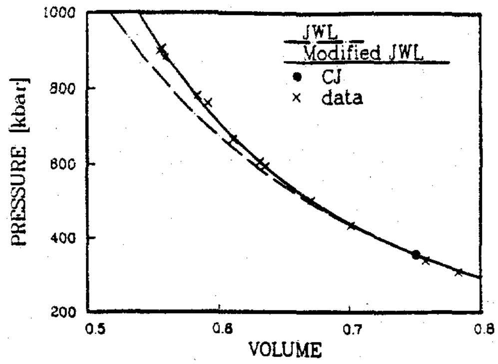

FIGURE 1. Hugoniot pressures.

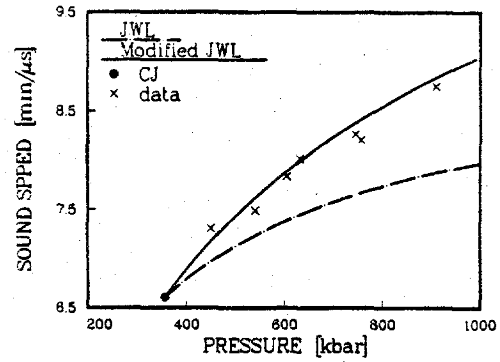

FIGURE 2. Sound Speeds.

JWL are given in Fig. 3. At this pressure level, both calculations give about the same pressures, but the one with modified JWL indicates a shorter overtaken time, an interval between the arrival of the detonation wave at the HE-window interface and the arrival of the release wave

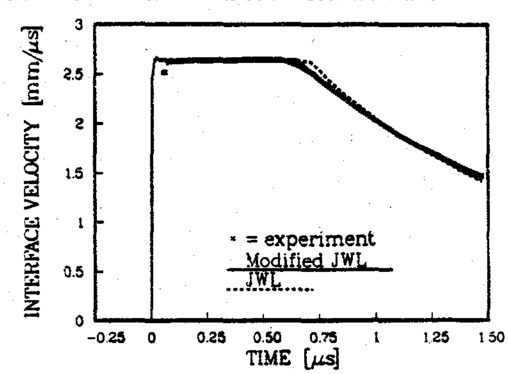

FIGURE 3. overdriven release experiment and simulations.

originated from the back of the flyer, as a result of a faster calculated sound speed and therefore matches the experiment better. Although in this example the improvement is minimal due to a very short HE charge length, we expect for larger systems, the impact from the sound speed correction can be quite significant.

CONCLUSIONS

Cylinder test alone is not sufficient to cover the overdriven regime for EOS calibration. Nor is the Hugoniot pressure only. More direct methods of measuring the Hugoniot properties, both pressure and sound speed, are available and should be used for the purpose. With the new treatment, we can expand the utility of the conventional JWL EOS to a higher pressure domain using the original set of parameters as a base. The simple modification takes advantage of the fact that the JWL EOS is already available in many hydrocodes and very little programming is required. The only additional information needed is the overdriven data.

ACKNOWLEDGEMENTS

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REFERENCES

1. E. L. Lee, H. C. Hornig, and J. W. Kury, Lawrence Livermore National Laboratory report UCRL-50422, 1968.
2. P. K. Tang, *J. Prop. Expl. Pyro.*, **22**, p. 45, 1997.
3. J. H. Kineke and C. E. West, Fifth Symposium (International) on Detonation, 1970, p. 533.
4. L. Green, E. Lee, A. Mitchel, and C. Tarver, Eighth Symposium (International) on Detonation, 1985, p. 587.
5. J. N. Fritz, R. S. Hixon, M. S. Shaw, C. E Morris, and R. G. McQueen, *J. App. Phys.*, to appear.
6. B. M. Dobratz, and P. C. Crawford, Lawrence Livermore National Laboratory report UCRL-52997, Change 2, 1985.
7. E. L. Baker, Tenth Symposium (International) on Detonation, 1993, p. 394.